



Research paper

The band offset, Half-metallic and optical behavior in the CrSb/KCl [0 0 1] interface: By DFT calculation

Arash Boochani^{a,*}, Elmira Sartipi^a, Shahram Solaymani^b

^a Department of Physics, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran

^b Young Researchers and Elite Club, West Tehran Branch, Islamic Azad University, Tehran, Iran

HIGHLIGHTS

- DFT has been applied to investigate the Half-metallic properties of CrSb/KCl [0 0 1].
- The optical response of CrSb/KCl [0 0 1] has been occurred at visible range.
- The band offset parameters at CrSb/KCl [0 0 1] interface are type I.

ARTICLE INFO

Keywords:

CrSb/KCl [0 0 1] interface

Band offset

Half-metallic property

Optical property

DFT

ABSTRACT

Half-metallic, optical and band offsets properties of CrSb/KCl [0 0 1] interface have been calculated within the density functional theory (DFT) framework using FP-LAPW+lo method. We found that the CrSb/KCl [0 0 1] heterojunction retain perfect half-metallic character with 0.95 eV and 1.5 eV spin flip gap at spin down, using GGA and mbj approximations, respectively. The 0.03 meV electrostatic potential gap between CrSb film and KCl substrate demonstrate that the CrSb film is the good spin electron source for injection to the KCl film. The optical coefficients such as real and imaginary parts of dielectric function, reflection, refraction, extinction and energy loss function indices have been shown the good optical response in the visible area. The band offset parameters of CrSb/KCl [0 0 1] interface are of the type-I model with great amount of Φ_B and χ potentials.

1. Introduction

The Giant Magneto Resistance (GMR) and Tunneling Magneto Resistance (TMR) discovery by Günberg [1] and Fert [2] opened the new windows to the magneto- electronic and spintronic industry. The ferromagnetic materials (FM) films are used for the spin source to the semiconductor films in the interfaces [3], but the spin polarization of the spin injection is very small, about 2% [4]. The Half-metallic ferromagnets were offered as a good candidate for this problem. The Half-metals have metallic behavior at majority spin and semiconducting behavior at the minority one which in ideal case have the 100% spin polarization. Some efforts on the dilute semiconductors such as GaMnAs have predicted spin-polarized electron sources with 90% efficiency but with very low Curie temperatures [5]. Also, some other works on the new Half-metals such as CrO₂ and La_{0.7}Sr_{0.3}MnO₃ have been done [6,7], but they all predict low Curie temperatures. Recently, the experimental and theoretical studies on the Heusler compounds have shown good Curie temperatures (above room temperature) [8,9]

but the Half-metallic property on their surface were decreased or vanished [10–12] and it was difficult to control the stoichiometry on the film surfaces [13]. The Akinaga's [14] work of predicting the Half-metallic behavior of CrAs in the zinc-blende (ZB) phase, opened the new windows to the binary compounds of Half metals which have two main phases, ZB and NiAs-type structures [15–17]. The crystal structure and nearly crystal lattice of these compounds with the III-V and II-VI semiconductors to minimize the interface spin scattering was the main cause to grow their films on the semiconductor substrates. But, the fabrication of Pnictides and chalcogenides in ZB structure has instability [18] and difficulty. Recently, some efforts on CrSb in the bulk, film and interface structures have been done both theoretically and experimentally [19–25]. According to the reports, CrSb ZB has the Half-metallic behavior by 3 μ_B magnetic moment and 2 eV spin flip gap at the Fermi level which indicates that this compound can be a good candidate for the spintronic and opto-electronic industry. But the results have shown that CrSb is meta-stable in the ZB bulk form, so a practical approach for stabilizing its ZB structure is the pseudomorphic growth of

* Corresponding author.

E-mail address: arash_bch@yahoo.com (A. Boochani).

<https://doi.org/10.1016/j.cplett.2018.10.068>

Received 5 August 2018; Received in revised form 9 October 2018; Accepted 28 October 2018

Available online 29 October 2018

0009-2614/ © 2018 Elsevier B.V. All rights reserved.

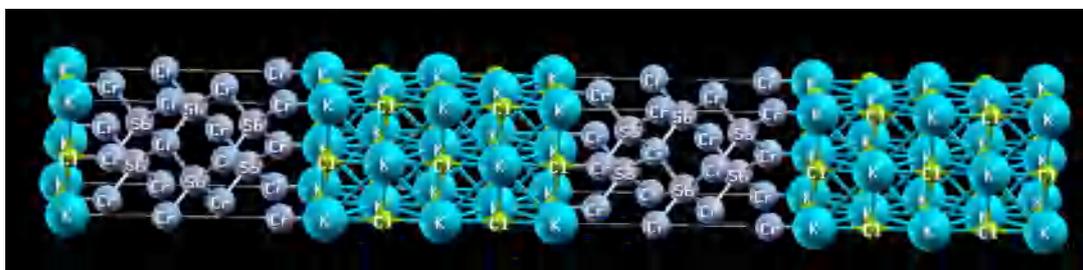


Fig. 1. The heterojunction picture of the CrSb/KCl [001].

Table 1

The layer distances of the CrSb/KCl [001] layers in Angstrom (Å) at two sides of the interface and comparison with CrSb and KCl bulk layers.

d_{CrSb}^{bulk}	$d_{CrSb}^{middlelayer}$	$d_{CrSb}^{subinterface-3thlayer}$	$d_{CrSb}^{interface-subinterface}$	$d_{interface}$	$d_{KCl}^{interface-subinterface}$	$d_{KCl}^{interface-3thlayer}$	$d_{CrSb}^{middlelayer}$	d_{KCl}^{bulk}
1.48	1.392	1.376	2.623	3.230	3.015	3.046	3.193	3.146

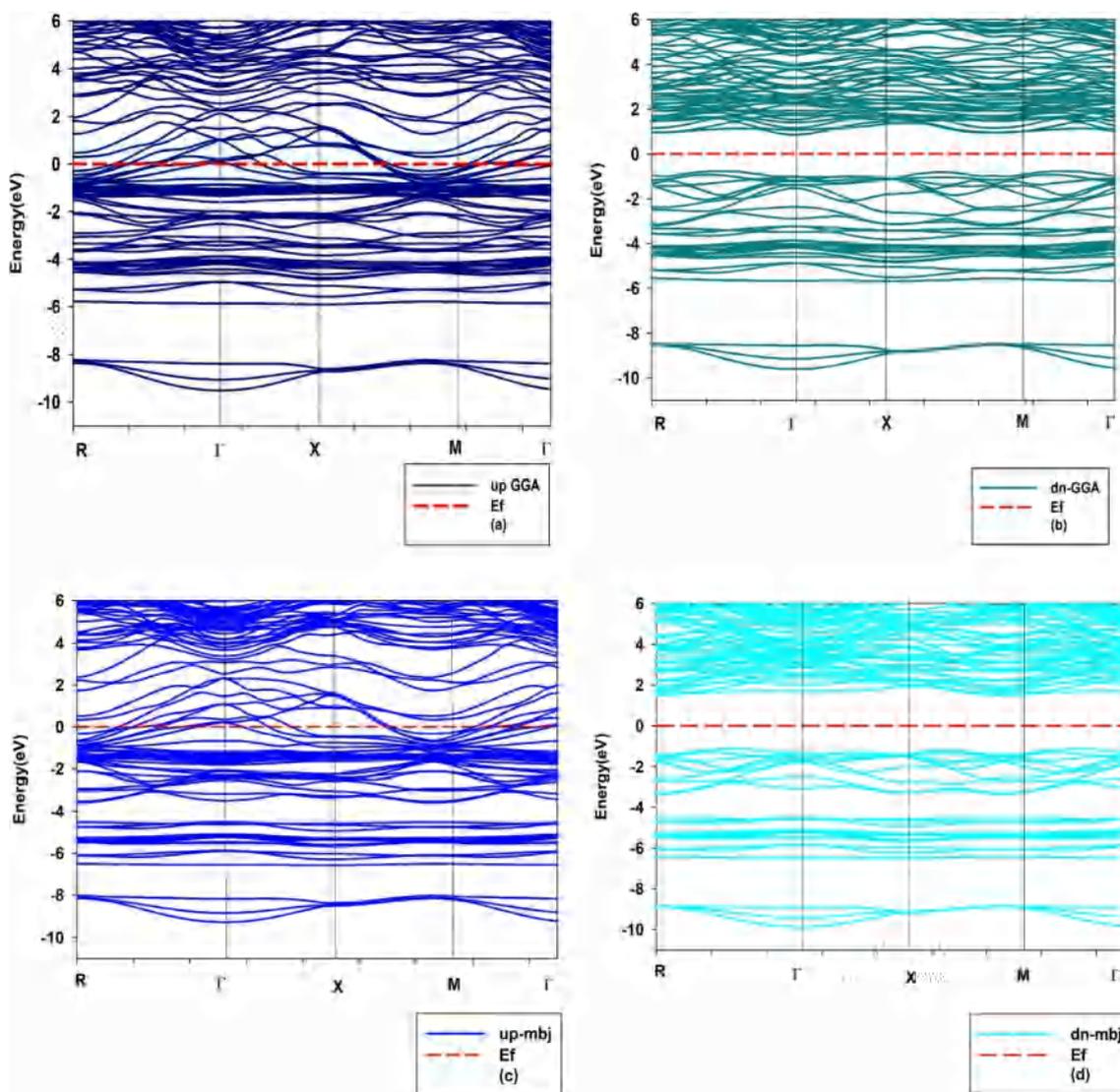


Fig. 2. The Bandstructure diagram of spin up and down versus the symmetry points at first brillouin zone for the GGA and mbj approximations.

CrSb thin film on ZB semiconductors such as GaAs, experimentally or GaSb and InAs, theoretically [26]. To selected the good substrate, there must be a negligible difference between the lattice constants of CrSb (6.14 Å) and its substrate (GaSb: 6.1 Å, InAs: 6.06 Å) [27]. Other

calculations have confirmed the meta-stability of CrSb ZB in the mechanical view by lower elastic constants and bulk modulus [28]. Growing the semiconductor substrates have difficulty in the experiment, so discovery of the new substrates which have accessibility,

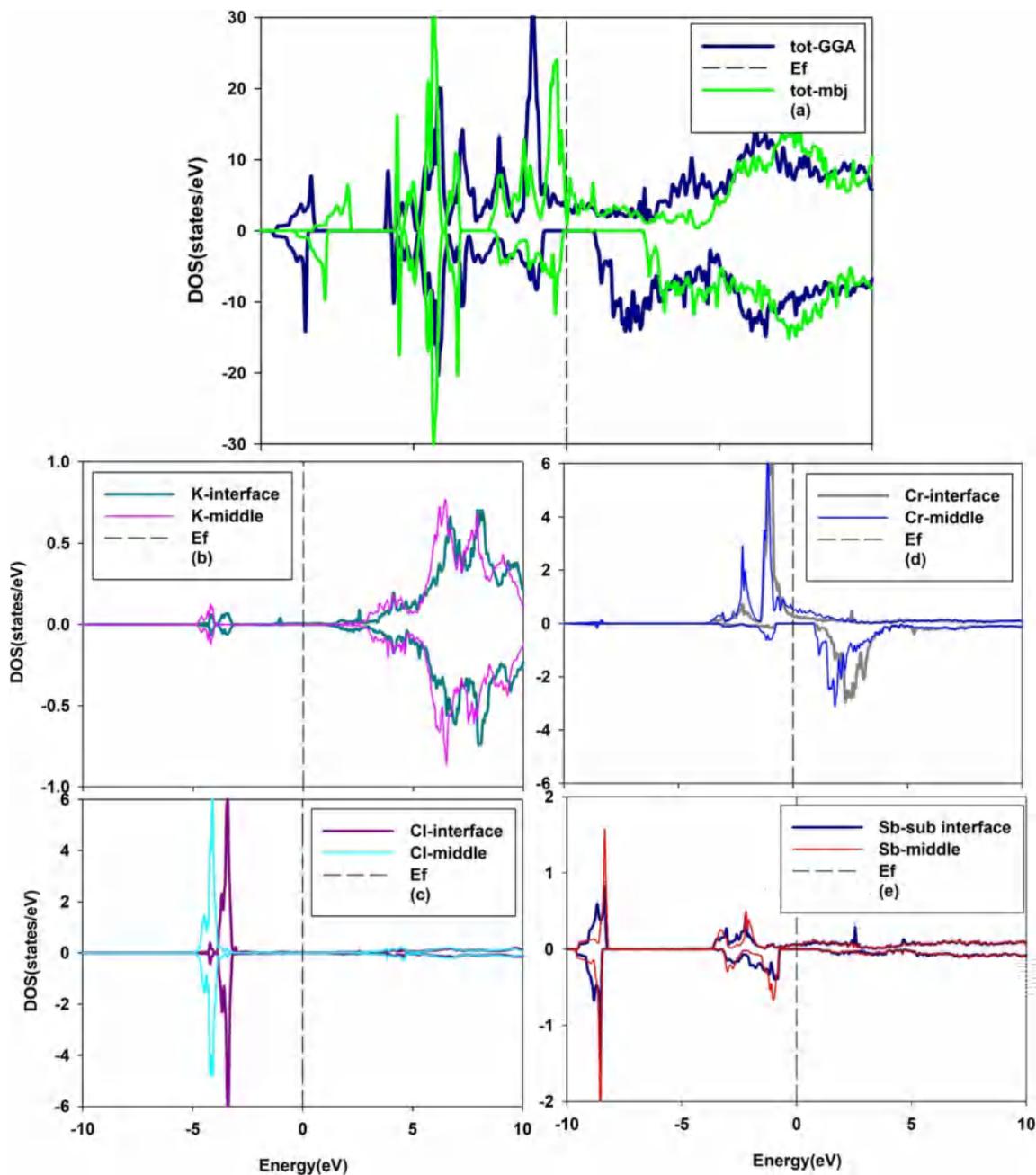


Fig. 3. (a) The total DOS of the CrSb/KCl [0 0 1] by GGA and mbj approximations, (b), (c) The K and Cl atoms DOS of the interface and middle layer by GGA, (d) The Cr DOS of the interface and middle layer by GGA, (e) The Sb DOS of the sub-interface and middle layer by GGA.

stability and affordability to keep the spin polarization at the interface is a necessity. The ionic compounds such as NaCl and KCl have the abovementioned properties for using in substrate of CrSb. Shandong et al [29] deposited CrSb on the KCl along the [0 0 1] direction by magnetron sputtering and reported the strong ferromagnetic behavior for this interface. Investigation of the important parameters for the spin injection such as the electronic and band alignment characteristics as well as optical properties can be interesting for opto-electronic applications but none of them have been reported yet.

2. Computational methods

The calculations have been done by the density functional theory (DFT) with full potential augmented plane waves plus local orbitals (FP-LAPW+lo) in the Wien2K code using the generalized gradient approximation (GGA) for exchange-correlation energy [30–32]. The

optimized input parameters such as KPoint, RKmax and l_{\max} for the CrSb/KCl [0 0 1] super lattice have been chosen as 500, 8.5 and 12, respectively, and the scf calculations were converged by electronic density to 0.0001. The atomic forces on their positions in Fig. 1 were optimized to 1 mRyd/a.u. with “mini-position” command. Also, the optical calculations were done by 1000 KPoint in the first Brillouin zone and random phase approximation (RPA) [33]. The film and substrate lengths were optimized in comparison with the middle atomic layers of the bulk layers and collected in Table 1 which shows little mismatch between them implying good accuracy of the atomic lengths at two sides of the interface. The CrSb/KCl [0 0 1] interface might be built in the two KCl-Cr and KCl-Sb geometries. For checking their stability, it can be calculate the cohesive energy (E_C) (Eq. (1)), which its negative amounts indicate thermodynamic stability. So, the E_C of the two mentioned interfaces of the CrSb/KCl [0 0 1], KCl-Cr and KCl-Sb were obtained by -6.1 eV and -0.5 eV, respectively, indicate good stability in

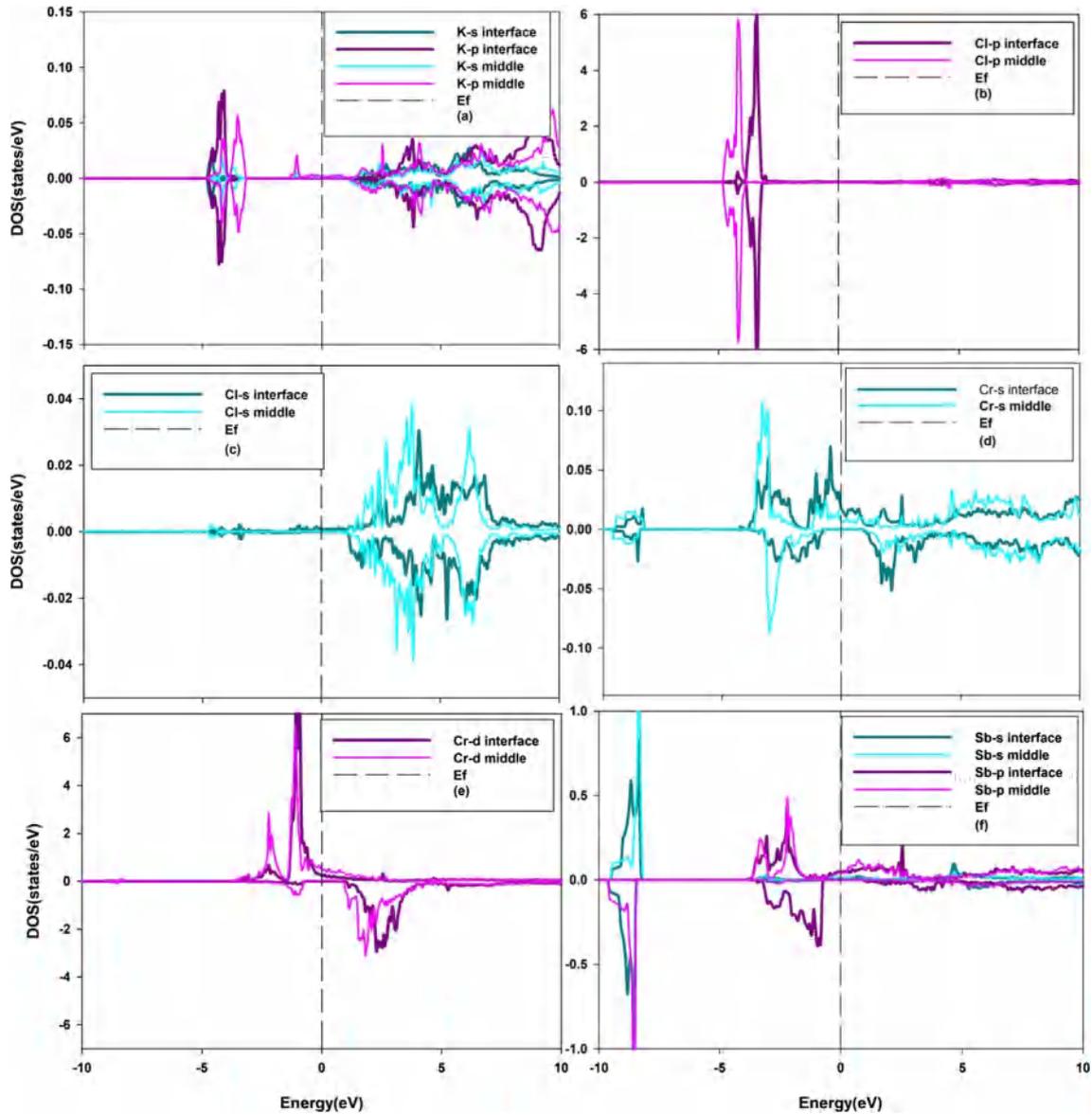


Fig. 4. The partial DOS of the valance and conduction orbitals of the Cr, Sb, K and Cl atoms.

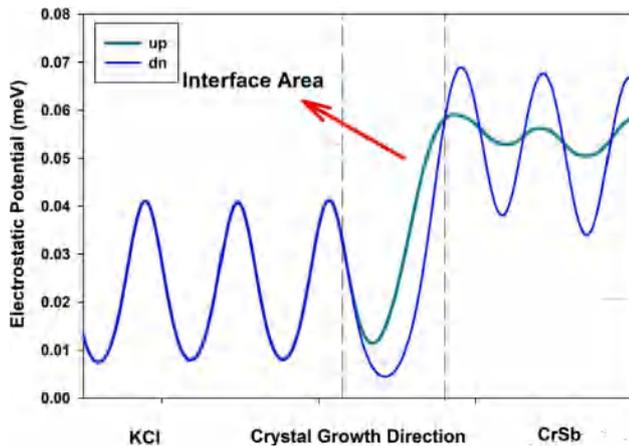


Fig. 5. The electrostatic potential along the CrSb/KCl [0 0 1] growth.

thermodynamic point of view for the KCl-Cr interface choice.

$$E_C = \frac{[E^{CrSb/KCl} - [N_{Cr}E_{Cr}^{Single} + N_{Sb}E_{Sb}^{Single} + N_K E_K^{Single} + N_{Cl}E_{Cl}^{Single}]]}{N_{Cr} + N_{Sb} + N_K + N_{Cl}} \quad (1)$$

In this relation, the $E^{CrSb/KCl}$ is the total energy of the CrSb/KCl [0 0 1] supercell, the E_{Cr}^{Single} , E_{Sb}^{Single} , E_K^{Single} and E_{Cl}^{Single} are the single atoms energies, respectively and N_{Cr} , N_{Sb} , N_K and N_{Cl} are the number of Cr, Sb, K and Cl atoms in the supercell.

3. Results and discussions

3.1. Electronic properties

Band structure (BS) diagram shows variation of the energy levels versus the K vectors in the first Brillouin zone and contains important information about the electronic, optical and transport behaviors of the matter. The BS of CrSb/KCl [0 0 1] interface is depicted in Fig. 2 for the up and down spins indicating the half-metallic behavior with 100% spin polarization at the Fermi level ($E_F = 0$) by GGA and mbj approximations. It is shown that the perfect spin-polarization at Fermi level is

Table 2

Total magnetic moment (TMM) and atomic magnetic moment (AMM) in terms of magneton-bohr (μ_B) of CrSb/KCl [0 0 1] heterojunction.

Approximation	TMM	Sb_{AMM}^{middle}	Cr_{AMM}^{middle}	$Sb_{AMM}^{sub-interface}$	$Cr_{AMM}^{interface}$	$K_{AMM}^{interface}$	$Cl_{AMM}^{interface}$	K_{AMM}^{middle}	Cl_{AMM}^{middle}
mbj	15.00	-0.206	3.133	-0.181	3.715	0.003	-0.003	0.000	0.000
GGA	15.00	-0.154	2.927	-0.136	3.578	0.010	0.009	0.000	0.000

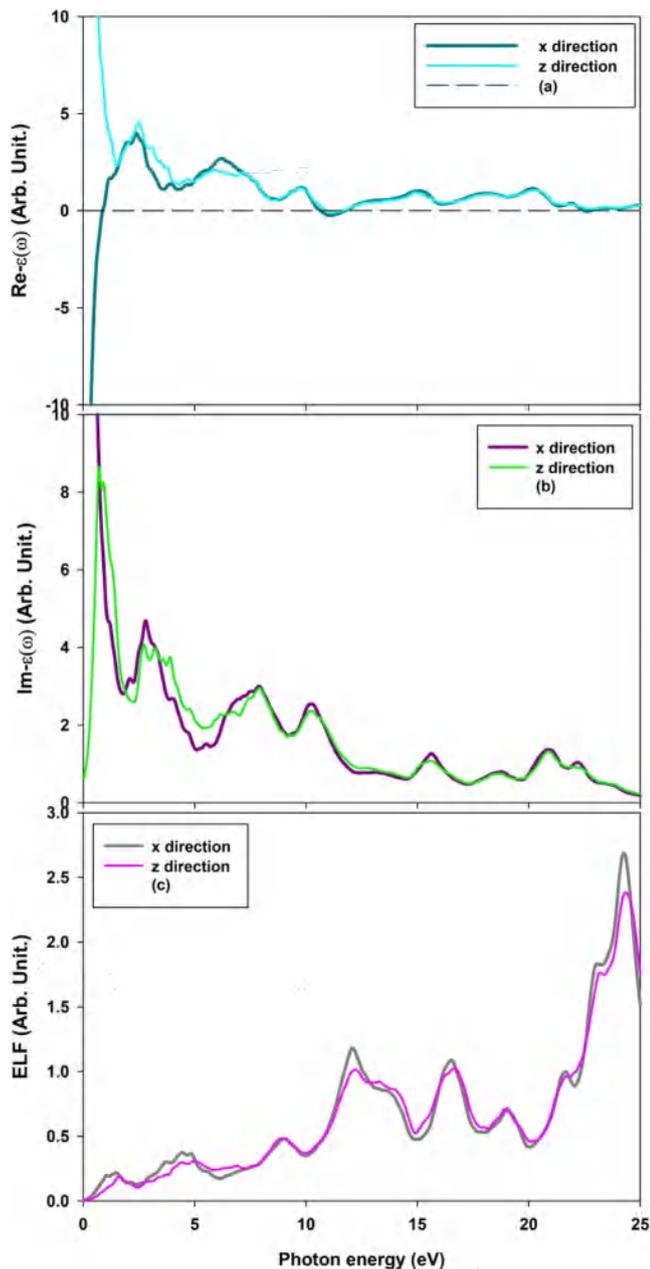


Fig. 6. (a), (b) The real part and imaginary part of dielectric function, (c) Energy Loss Function (ELF) versus photon energy at x and z directions.

existed for the two mentioned approximations, at spin up no significant changes have taken place but the energy and spin flip gaps were increased of 1.68 eV, 0.94 eV–1.5 eV and 2.6 V, respectively and emerged a gap around the -4eV area. Furthermore, it has complete magnetic behavior by metallic and semiconducting behavior for the up and down spins, respectively. The Fermi level lies in the middle gap while the conduction band minimum (CBM) resides at Γ and the valance band maximum (VBM) points appear at $R \rightarrow \Gamma$, $X \rightarrow M$, $M \rightarrow \Gamma$ directions in the two mentioned approximations. Curvature of the up spin curves

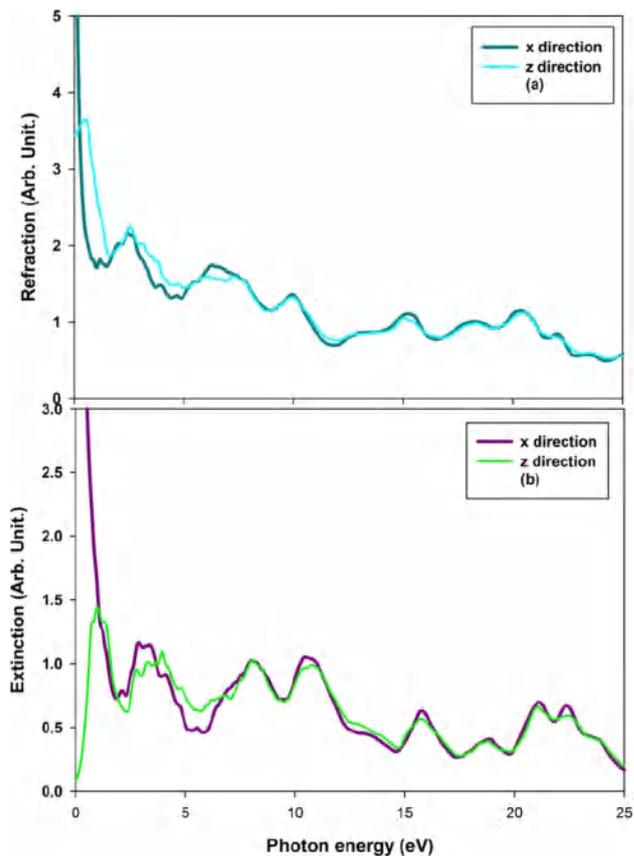


Fig. 7. (a) The refraction and (b) The extinction coefficients diagrams of x and z directions.

above the Fermi level are very higher than down ones which implies the great electron mobility at this levels, therefore, CrSb/KCl [0 0 1] heterojunction can be a good candidate for GMR and TMR applications. Comparison of the BS and density of states (DOS) graphs in Fig. 3 reveals that the main spin polarization at the Fermi level is due to the Cr-d and Sb-p interactions. For better comparisons, the total DOS diagram by mbj approximation is added to the Fig. 3(a), confirming the 100% spin-polarization and perfect half-metallic nature of the CrSb/KCl [0 0 1] heterojunction. Also, inhomogeneous atomic bonds around the interface are other reasons for this subject. As demonstrated in Fig. 3, because of the Cr-K bonds at the interface, the DOS amount of the interface Cr decreases at the energy of -3eV compared to the middle one. The partial DOS diagrams of Fig. 4 have been shown that the Cr-d and Sb-p orbitals in the -5 eV to 0 eV are the main electron source injection to the K-p, Cl-s and Sb-p orbitals. Also, it is clear that K and Cl orbitals have no any contribution at conduction. Displayed in Fig. 5 for the up and down spins are the changes of the electrostatic potential energy of the substrate and film layers versus the growth direction. It is clear that the electrostatic potential energy of both spins are the same for the substrate layer (KCl) but different for the film sides such that the electrostatic potential energy of the down spin is greater than up one and hence, the majority charge carriers belong to the up spin, so, by changing the external magnetic field the spin injection can be controlled. Also, the potential difference at the interface area is valuable

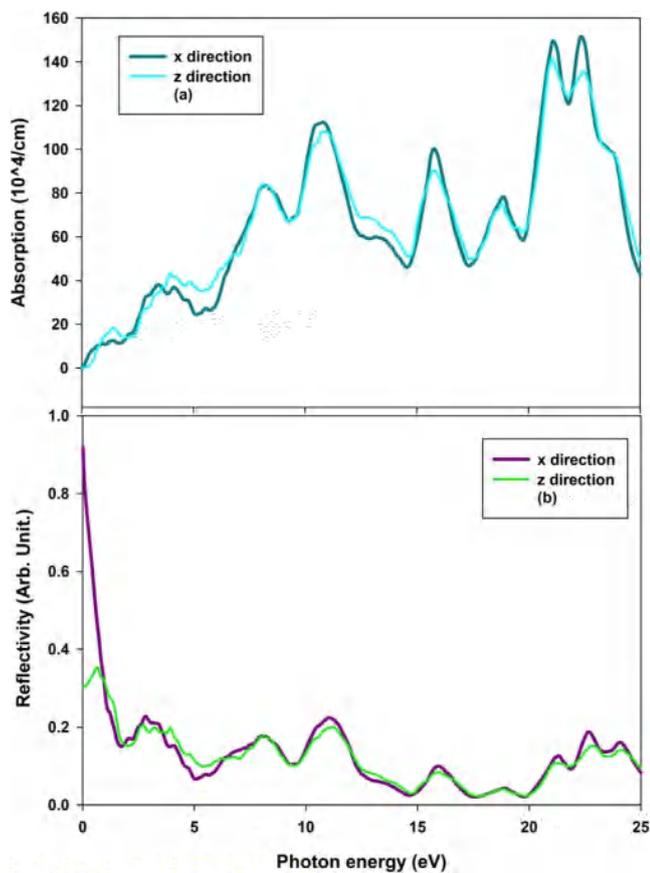


Fig. 8. (a) Absorption (b) Reflectivity curves at x and z directions.

Table 3

Schottky barrier Φ_B (eV), electron affinity (χ), VBO and CBO for the CrSb/KCl [0 0 1] and other interfaces.

	Φ_B (eV)	χ (eV)	χ (eV)	VBO	CBO
CrSb/KCl	4.66	CrSb = 5.25	KCl = 3.44	3.68	1.81
MoS ₂ /Al ₂ O ₃ ⁴²	–	–	Al ₂ O ₃ = 4.10	3.41	–
HfO ₂ /GaN ⁴³	3.3	GaN = 3.0	HfO ₂ = 2.5	–0.1	2.5
MgO/GaN ⁴⁴	–	–	GaN = 1.06	3.3	–
P-Si/InN ⁴⁵	–	InN = 5.8	P-Si = 4.05	1.39	1.81
VSb/GaSb ¹⁵	0.51	–	–	1.25	0.47

because the film side potentials of about 0.03 meV can help on better switching of the electron injection. The identical spin behaviors in the substrate layer provides a good meter for analyzing the electron injection of various spins and thus it is a privilege for KCl to be selected as a sub-layer.

The total and intrinsic magnetic moments of CrSb/KCl [0 0 1] supercell and important layers have been reported in Table 2. It is shown that the total magnetic moment (TMM) for the GGA and mbj approximations are equal to 15.00 μ_B indicating no change in the TMM, which implies to accuracy in our calculations. The integer and high amounts of TMM with two mentioned approximated have been shown the perfect half-metallic property and strong ferromagnetic behavior for CrSb/KCl [0 0 1] heterojunction in agree by our electronic calculations and experiment [29]. The comparison atomic magnetic moment (AMM) of layers were indicated the magnetic moments of K and Cl are zero in the middle layer of KCl and by approaching to the interface are raised and on the other side of the interface, the Cr magnetic moment were increased at interface than middle layers on the contrary the Sb ones have been decreased in the sub-interface layer.

3.2. Optical properties

The matter response to the optical beam is explained by the dielectric tensor which is a combination of two parts, the real and imaginary dielectric functions ($Re-\epsilon(\omega)$ and $Im-\epsilon(\omega)$) whilst based on the Kramers-Kroing relations the other optical coefficients such as refraction, reflection, energy loss function (ELF), extinction and absorption indices are extracted from the dielectric function. $Re-\epsilon(\omega)$ of the CrSb/KCl [0 0 1] is depicted in Fig. 6(a) in the two x and z directions (with being x-y plane and the growth direction). Obviously, after 3 eV behaviors are quite similar in both directions, but in the infrared (IR) region they have different trends. The static amounts of the $Re-\epsilon(\omega)$ ($Re-\epsilon(0)$) have shifted towards the negative and positive infinity respectively, implying the metallic behavior at x direction. According to Fig. 8(b), $Im-\epsilon(\omega)$ diagrams start from zero at z direction but has infinite amount in x direction. Each $Im-\epsilon(\omega)$ peak explains an electron transmission from a full level to an empty one, as a result of the inter + intra band transitions in metals. The plasmonic oscillations occur at 7 eV and 11.5 eV at x direction, corresponding to the $Re-\epsilon(\omega)$ roots and sharp reduction of $Im-\epsilon(\omega)$ as well as the appearance of ELF peaks in these photon energies. Increasing the photon energy is followed by reduction of the $Re-\epsilon(\omega)$ and $Im-\epsilon(\omega)$ but the rise of the ELF curves, so the CrSb/KCl [0 0 1] interface has good efficiency in the IR and visible ranges.

Another optical parameter portrayed in the Fig. 7(a) is the refraction index for the x and z directions. Apparently, it decreases by increasing the photon energy, representing an insulator at the UV area and the amounts of lower than one between the energies of 10–15 eV imply the superluminal phenomena. However, dual behavior is observed in the IR range, that is, while the static amount of the refraction index goes towards huge values in x direction inferring a metallic nature, it has a finite small amount in the z direction suggesting a the semiconducting property. The extinction indices of the CrSb/KCl [0 0 1] have been depicted in Fig. 6(b) for the two x and z directions. Clearly, they have asymmetric behavior in lower energies but homogenous manner at the UV area. At higher energies in the two mentioned directions, reduction rate of the absorption amplitude is low and thus the optical transmission would be great.

The plots of absorption indices in the two x and z directions in Fig. 8(a) indicate a close similar trend at all energy regions and have been growth by increasing photon energy. In reference to the absorption and reflection figures, increase of the absorption and decrease of the reflection amounts at higher energies emphasize the transparency of the CrSb/KCl [0 0 1] interface at both directions, but in the IR region and visible edge the directional behaviors are opposite. Reflectivity is a function of the incident photon direction in the IR area with two different optical behaviors, metallic and semiconducting, in the x and z directions respectively.

3.3. Band offsets of CrSb/KCl [0 0 1] interface

The band alignment parameters are technologically related quantities in the electronic transportations. Generally, a halfmetal/semiconductor heterojunction in the majority spin simulates a metal/semiconductor contact with a p- or n-type Schottky barrier (Φ_B), while in the minority spin this interface acts as a semiconductor/semiconductor heterojunction and the band discontinuities are defined as the valence and conduction band offsets (VBO, CBO). Φ_B are defined as the difference between the semiconductor valance band maximum VBM (conduction band minimum (CBM)) and metal Fermi level, while VBO (CBO) is the difference between minority halfmetal VBM (CBM) and semiconductor VBM (CBM). Clearly, seeking the new interface compounds for the spintronic, optoelectronic and magneto-resistances applications is a necessary. Accordingly, the band alignment parameters of the CrSb/KCl [0 0 1] VBO and CBO have not been reported so far. The spin injection and transportation mechanisms are functions of the band offsets at the interface films such as VBO and CBO and their

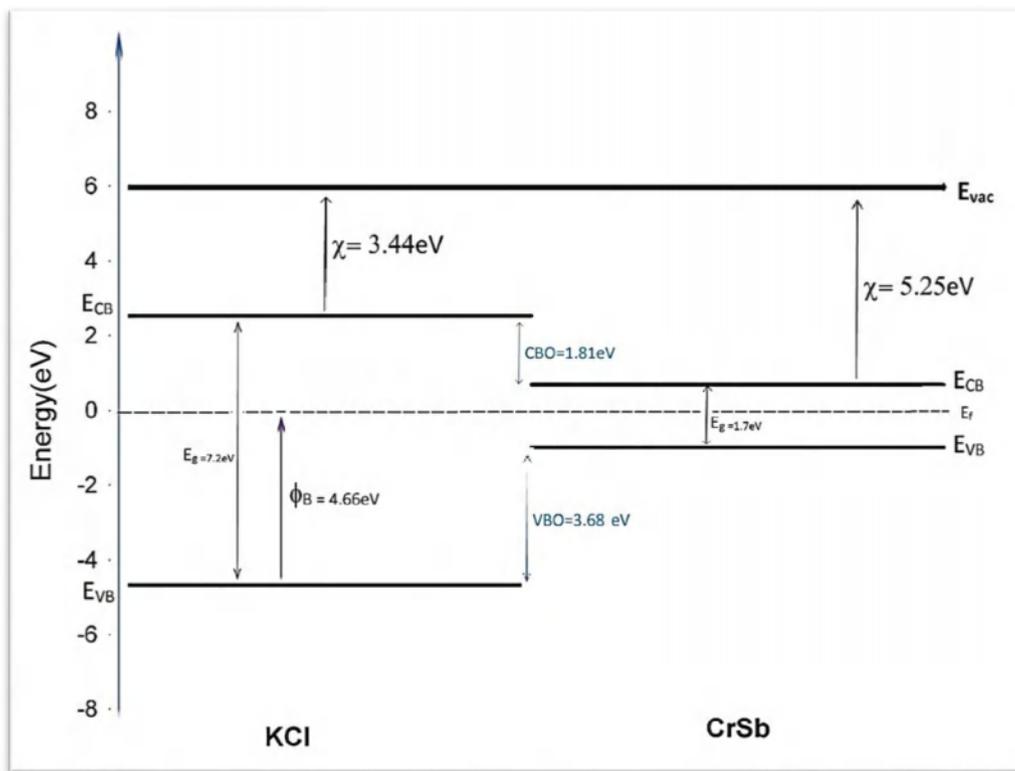


Fig. 9. The schematic band alignment at CrSb/KCl [001] heterojunction.

relative parameters. Referring to the Kraut [33] relations, the band offsets can be calculated by [34]:

$$\Delta E_V(\text{CrSb/KCl}) = E_{VB}(\text{CrSb}) - E_{VB}(\text{KCl}) \quad (1)$$

$$\Delta E_C(\text{CrSb/KCl}) = E_g(\text{CrSb}) - E_g(\text{KCl}) - \Delta E_V \quad (2)$$

Having been extracted based on the above relations, the band offsets and their related parameters such as the Schottky barrier Φ_B (eV), electron affinity (χ), VBO and CBO of the CrSb/KCl [001] have been listed in Table 3 and compared with some other interfaces. As illustrated in Fig. 9, CrSb/KCl [001] interface is of type I (straddling gap) namely that the valance and conduction edges of CrSb lie in the KCl gap. In conclusion, the CrSb/KCl [001] band alignment is a good candidate for the Quantum wells emission (TMD) [35,36], tunneling diodes and FET applications [37–45].

4. Conclusion

Based on the DFT calculations by GGA approximation, we found good stability for CrSb/KCl [001] heterojunction in the energy view. Our results indicated perfect half-metallic behavior by 0.95 eV spin flip gap at spin down whereas the electrons have high mobility at spin up and low at down one. The main reason of the energy gap at the Fermi level is the *Cr-d* and *Sb-p* interaction. Also the electrostatic potential indicated the great potential difference at the interface area which made the CrSb/KCl [001] heterojunction for the spin injection applications. The optical response at the IR region is metallic at *z* direction but no optical transmission has been occurred at this area. The main optical response of CrSb/KCl [001] has been occurred at visible range and at high photon energy, most light passes through of this matter.

Our calculations indicated the type-I model of the band offset levels at the CrSb/KCl [001] interface location with great Φ_B and χ potentials. According to the great energy gap of KCl and the band alignment parameters this heterojunction can be a good candidate for GMR and TMR applications. The important note is the easy growth of the KCl

than other conventional semiconductors for the substrate.

Competing interests

The authors declare that they have no competing interests.

Acknowledgments

This work is resulted from a scientific research in the Kermanshah Branch, Islamic Azad University.

References

- [1] G. Binasch, P. Grunberg, F. Saurenbach, W. Zinn, Phys. Rev. B 39 (1989) 4828.
- [2] O. Bengone, O. Eriksson, J. Fransson, I. Turek, J. Kudrnovský, V. Drchal, Phys. Rev. B 70 (2004) 035302.
- [3] R.A. de Groot, F.M. Mueller, P.G. van Engen, K.H.J. Buschow, Phys. Rev. Lett. 50 (1983) 2024.
- [4] H.J. Zhu, M. Ramsteiner, H. Kostail, M. Wassermeier, et al., Phys. Rev. Lett. 87 (2001) 016601.
- [5] Y. Onhno, D.K. Young, B. Beschoten, F. Matsukara, H. Ohno, D.D. Awschalom, Nature (London) 402 (1999) 790.
- [6] R.J. Soulen Jr, J.M. Byers, M.S. Osofsky, B. Nadgorny, et al., Science 282 (1998) 85.
- [7] J.H. Park, E. Vescovo, H.J. Kim, C. Kwon, R. Ramesh, T. Venkatesan, Nature (London) 392 (1998) 794.
- [8] F. Ahmadian, A. Boochani, Physica B 406 (14) (2011) 2865.
- [9] H. Lashgari, M.R. Abolhassani, A. Boochani, E. Sartipi, R. Taghavi-Mendi, Indian J. Phys. 90 (8) (2016) 909.
- [10] H. Akinaga, M. Mizuguchi, J. Phys.: Condens. Matter 16 (2004) S5549.
- [11] I. Galanakis, S. Ostanin, M. Alouani, H. Dreysse, J.M. Will, Phys. Rev. B 61 (2000) 4093.
- [12] (a) G.A. Wijs, R.A. de Groot, Phys. Rev. B 64 (2001) R020402; (b) I. Galanakis, J. Phys. Condens. Matter 14 (2002) 6329.
- [13] (a) D. Ristoiu, J.P. Nozieres, C.N. Borca, et al., Europhys. Lett. 49 (2000) 624; (b) D. Ristoiu, J.P. Nozieres, et al., Appl. Phys. Lett. 76 (2000) 2349.
- [14] H. Akinaga, T. Manago, M. Shirai, Jpn. J. Appl. Phys. 39 (2000) L1118.
- [15] A. Boochani, M.R. Abolhasani, M. Ghoranneviss, M. Elahi, Commun. Theor. Phys. 54 (1) (2010) 148.
- [16] E. Sartipi, A. Hojabri, A. Bouchani, M.H. Shakib, Chin. J. Chem. Phys. 24 (2) (2011) 155.
- [17] M. Shirai, Physica E 10 (2001) 143.

- [18] Y. Zaho, A. Zunger, *Phys. Rev. B* 71 (2005) 132403.
- [19] J.H. Zhao, F. Matsukura, K. Takamura, E. Abe, D. Chiba, H. Ohno, *Appl. Phys. Lett.* 79 (2001) 2776.
- [20] B.G. Liu, *Phys. Rev. B* 67 (17) (2003) 172411.
- [21] J.E. Pask, L.H. Yang, C.Y. Fong, W.E. Pickett, S. Dag, *Phys. Rev. B* 67 (22) (2003) 224420.
- [22] M. Regus, G. Kuhn, S. Mankovsky, H. Ebert, W. Bensch, *J. Solid State Chem.* 196 (2012) 100.
- [23] Li Shandong, Lü Liya, Huang Zhigao, *J. Magn. Magn. Mater.* 312 (2) (2007) 305.
- [24] I. Galanakis, S.G. Pouliasis, *J. Magn. Magn. Mater.* 321 (8) (2009) 1084.
- [25] M.S. Miao, Walter R.L. Lambrecht, *Phys. Rev. B* 71 (2005) 064407.
- [26] F. Ahmadian, M.R. Abolhassani, M. Ghoranneviss, M. Elahi, *Physica B* 404 (20) (2009) 3684.
- [27] B.-G. Liu, *Phys. Rev. B* 67 (2003) 172411.
- [28] S. Rezaee, A. Boochani, M. Majidiyan, A. Ghaderi, S. Solaymani, M. Naseri, *Rare Met.* 33 (5) (2014) 615.
- [29] L. Shandong, T. Zongjun, F. Jianglin, D. Jenq-Gong, L. Kai-Xin, H. Zhigao, H. Yinhu, D. Youwei, *Solid State Commun.* 149 (2009) 196.
- [30] J. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 77 (1996) 3865.
- [31] (a) P. Hohenberg, W. Kohn, *Phys. Rev.* 136 (1964) 864;
(b) W. Kohn, L.J. Sham, *Phys. Rev. A* 140 (1995) 1133.
- [32] P. Blaha, K. Schwarz, P. Sorantin, S.B. Trickey, *Comput. Phys. Commun.* 59 (1990) 399.
- [33] R.L. Kronig, *J. Opt. Soc. Am.* 12 (1926) 547.
- [34] E.A. Kraut, R.W. Grant, J.R. Waldrop, S.P. Kowalczyk, *Phys. Rev. Lett.* 44 (1980) 1620.
- [35] R.L. Anderson, *IBM J. Res. Dev.* 4 (3) (1960) 283.
- [36] N. Naghavi, D. Abou-Ras, N. Allsop, N. Barreau, S. Bücheler, et al., *Prog. Photovoltaics* 18 (2010) 411.
- [37] C. Bugot, N. Schneider, M. Bouttemy, A. Etcheberry, D. Lincot, F. Donsanti, *Thin Solid Films* 582 (2015) 340.
- [38] Y.-H. Lee, X.-Q. Zhang, W. Zhang, M.-T. Chang, et al., *Adv. Mater.* 24 (2012) 2320.
- [39] Y. Zhan, Z. Liu, S. Najmaei, P.M. Ajayan, J. Lou, *Small* 8 (2012) 966.
- [40] E. Hazrati, S.J. Hashemifar, H. Akbarzadeh, *J. Appl. Phys.* 140 (2008) 113719.
- [41] R.Q. Wu, G.W. Peng, Y.P. Feng, *J. Phys. Conf. Ser.* 29 (2006) 150.
- [42] L. Xinke, H. Jiazhu, T. Dan, et al., *J. Alloy. Compd.* 650 (2015) 502.
- [43] T.E. Cook, C.C. Fulton, W.J. Mecoouch, R.F. Davis, *J. Appl. Phys.* 94 (2003) 7155.
- [44] R. Basanta, K. Mahesh, K.R. Mohana, N.B. Thirumaleshwara, S.B. Krupanidhi, *J. Phys. D: Appl. Phys.* 48 (2015) 423001.
- [45] T.N. Bhat, M. Kumar, M.K. Rajpalke, B. Roul, N. Sinha, S.B. Krupanidhi, *J. Appl. Phys.* 109 (2011) 123707.